

# **Certificate of Analysis**

Print Date: May 18th 2020

www.tocris.com

Product Name: JBJ-03-142-02 Catalog No.: 6962 Batch No.: 1

CAS Number: 2068806-31-3

IUPAC Name: (4-Fluorophenyl)methyl N-[2-[(1-methyl-1*H*-pyrazol-4-yl)amino]-4-pyrimidinyl]-N-[3-[(1-oxo-2-propen-1-yl)amino]

phenyl]carbamate

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>25</sub>H<sub>22</sub>FN<sub>7</sub>O<sub>3</sub>

**Batch Molecular Weight:** 487.5

Physical Appearance: White solid

Solubility: DMSO to 50 mM Storage: Store at -20°C

**Batch Molecular Structure:** 

## 2. ANALYTICAL DATA

**HPLC:** Shows 99.6% purity

<sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 61.6 4.55 20.11 Found 61.27 4.57 20.01



## **Product Information**

Print Date: May 18th 2020

www.tocris.com

Product Name: JBJ-03-142-02 Catalog No.: 6962 Batch No.: 1

CAS Number: 2068806-31-3

IUPAC Name: (4-Fluorophenyl)methyl N-[2-[(1-methyl-1*H*-pyrazol-4-yl)amino]-4-pyrimidinyl]-N-[3-[(1-oxo-2-propen-1-yl)amino]

phenyl]carbamate

#### **Description:**

Highly potent epidermal growth factor receptor (EGFR) and ErbB2 (human epidermal growth factor receptor; HER2) inhibitor. Inhibits wild type and tumorgenic mutated receptors (exon 20 insertion; Ex20Ins). Antiproliferative in vitro (IC $_{50}$  values are 7.6, 30 - 95, 3.8 and 19 - 31 nM for Ba/F3 cells expressing wild type EGFR, EGFR with Ex20Ins mutation, wild type HER2 and HER2 with Ex20Ins mutation, respectively). Also inhibits other common EGFR mutants. Antiproliferative in patient-derived lung cancer cell lines.

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>25</sub>H<sub>22</sub>FN<sub>7</sub>O<sub>3</sub>

Batch Molecular Weight: 487.5 Physical Appearance: White solid

Minimum Purity: ≥98%

#### **Batch Molecular Structure:**

Storage: Store at -20°C

### Solubility & Usage Info:

DMSO to 50 mM

## **Stability and Solubility Advice:**

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

#### **Licensing Information:**

Sold under license from Dana-Farber Cancer Institute

References:

**Jang** *et al* (2018) Discovery of a highly potent and broadly effective epidermal growth factor receptor and HER2 exon 20 insertion mutant inhibitor. Angew.Chem.Int.Ed.Engl. *57* 11629. PMID: 29978938.